EUROPHYSICS LETTERS 15 May 2000

Europhys. Lett., **50** (4), pp. 540–546 (2000)

Inhomogeneity-induced superconductivity?

J. Eroles[1,2], G. Ortiz[1], A. V. Balatsky[1] and A. R. Bishop[1]

[1] *Theoretical Division, Los Alamos National Laboratory - Los Alamos, NM 87545, USA*
[2] *Centro Atómico Bariloche and Instituto Balseiro - S. C. de Bariloche, Argentina*

(received 28 February 2000; accepted 3 March 2000)

PACS. `74.20.-z` – Theories and models of superconducting state.
PACS. `74.20.Mn` – Nonconventional mechanisms (spin fluctuations, polarons and bipolarons, resonating valence bond model, anyon mechanism, marginal Fermi liquid, Luttinger liquid, etc.).
PACS. `71.27.+a` – Strongly correlated electron systems; heavy fermions.

Abstract. – A t-J–like model for inhomogeneous superconductivity of cuprate oxides is presented, in which local anisotropic magnetic terms are essential. We show that this model predicts pairing, consistent with experiments, and argue how the macroscopic phase-coherent state gradually grows upon lowering of the temperature. We show that appropriate inhomogeneities are essential in order to have significant pair binding in the thermodynamic limit. Particularly, *local* breaking of $SU(2)$ spin symmetry is an efficient mechanism for inducing pairing of two holes, as well as explaining the magnetic scattering properties. We also discuss the connection of the resulting inhomogeneity-induced superconductivity to recent experimental evidence for a linear relation between magnetic incommensurability and the superconducting transition temperature, as a function of doping.

There is a growing body of experimental evidence suggesting that the superconducting state in cuprate oxides is "inhomogeneous", such that the locally defined charge density varies across the sample in the ground state. Spatially inhomogeneous features in the spin and charge channels have been indicated in a number of experiments on high-T_c materials [1–6]. The simplest realization of this state is the so-called "stripe" phase where charges cluster in nanoscale linear patterns and the remainder of the sample is essentially an antiferromagnetically correlated insulator. This represents a nanoscale distribution of charge and spin, rather than a global phase separation. These experiments lead us to a central question: Is the superconducting state found in high-T_c cuprates inhomogeneous as a result of spin/charge inhomogeneities? We believe that the answer to this question is yes. Moreover, we argue that spatial spin/charge inhomogeneities are in fact *necessary* for pairing and subsequent formation of the superconducting state in these compounds. This situation should be contrasted with the case of conventional superconductors, resolved by the BCS (Bardeen-Cooper-Schrieffer) theory, that starts with a homogeneous metallic state and describes the formation of a homogeneous superconducting state. It is commonly believed that magnetic correlations, characterized by the spin exchange energy $J \sim 1500\,\mathrm{K}$ are responsible for the pairing interactions in the cuprates and are, therefore, crucial for our inhomogeneous exchange approach. Moreover, the existence of a spin gap has been experimentally proven [7]. A model that naturally incorporates these features (inhomogeneities, magnetism and spin gap) is a t-J–like model with explicitly broken spatial and magnetic symmetries.

Of central importance for the present work is a microscopic model which captures the main low energy physics of doped antiferromagnetic (AF) Mott insulators. In particular, we show that our minimal model properly describes the magnetic properties observed in a wide variety of doped cuprate oxide materials. The key ingredient is the existence of magnetic perturbations which explicitly break *local* spin-rotational invariance (*e.g.*, due to local spin-orbit coupling [8]) and thereby induce substantial hole pair binding. We then develop a mean-field theory of superconductivity based upon a phenomenology from our microscopic model. We emphasize that in our approach there are two, in principle different, energy scales; one associated to the pairing of holes and another related to the phase coherence of the pairs (that establishes T_c). Basically the inhomogeneities induce a strong hole pairing, which in turn Josephson-tunnels coherently between stripes, separated by insulating AF regions, phase-locking into a macroscopic supercurrent superfluid stiffness. Recently, a simple linear relation between the superconducting transition temperature T_c and the AF incommensuration δ has been observed for the LSCO [3] and YBCO [4] high-T_c compounds: $k_\mathrm{B}T_\mathrm{c} \propto \delta$, where k_B is the Boltzman constant. We find that for this relation to hold we need a power law Josephson tunneling.

Microscopic model. – Our model Hamiltonian describing the low energy dynamics of CuO_2 planes is $H = H_{t\text{-}J} + H_\mathrm{inh}$, where the background Hamiltonian $H_{t\text{-}J}$ is the standard t-J model,

$$H_{t\text{-}J} = -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + J \sum_{\langle i,j\rangle} \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \frac{1}{4}\bar{n}_i \bar{n}_j \right) . \tag{1}$$

For the inhomogeneous component, we take

$$H_\mathrm{inh} = \sum_{\langle \alpha,\beta\rangle} \delta J_z \; S^z_\alpha S^z_\beta + \frac{\delta J_\perp}{2} \left(S^+_\alpha S^-_\beta + S^-_\alpha S^+_\beta \right) ,$$

with $\delta J_\perp \neq \delta J_z$, representing the magnetic perturbation of a static local Ising anisotropy, locally lowering spin symmetry. Here $\langle i,j\rangle$ are near-neighbor sites, while $\langle \alpha,\beta\rangle$ are two near-neighbor sites characterizing the bonds that are perturbed and where $SU(2)$ spin-rotational invariance is explicitly broken. The network of perturbed bonds form mesoscopic patterns determined by the distribution of stripe segments. The spin-$\frac{1}{2}$ operator $\boldsymbol{S}_i = \frac{1}{2} c^\dagger_{i\sigma} \boldsymbol{\tau}_{\sigma\sigma'} c_{i\sigma'}$, the electron occupation number $\bar{n}_i = c^\dagger_{i\uparrow}c_{i\uparrow} + c^\dagger_{i\downarrow}c_{i\downarrow}$, and $c^\dagger_{i\sigma}(c_{i\sigma})$ creates (annihilates) an electron of spin σ in a Wannier orbital centered at site i; $\boldsymbol{\tau}$ are the 3 Pauli matrices. This is a three-state model with the hopping constrained to the subspace with no doubly occupied sites. In the following, all energies will be measured in units of J.

Our modeling strategy consists in assuming the existence of an inhomogeneous mesoscopic skeleton of stripe segments [9], and then exploring its consequences, mainly the competition between magnetism and superconductivity. We do not address here the important problem of the formation and stability of this skeleton morphology. The origin(s) of "stripe segment" formation in high-temperature superconductors is as yet unclear and several physical mechanisms could act cooperatively and be responsible for the generation of multiple length scales, among them: spin-orbit coupling, local Jahn-Teller distortions induced by the hole, effective interactions coming from a multi-band Hubbard Model (HM) (including explicitly the oxygen and copper bands), oxygen buckling at the stripe, and other local magnetoelastic effects [10]. Competitions between attractive short range forces and repulsive long range ones can certainly spontaneously break translational and/or rotational invariance in the CuO_2 planes [11,12], but this is not necessarily the only mechanism. However, we show below that the mere existence of appropriate *local* magnetic anisotropies is crucial for pair-formation.

We start by showing that, as far as we could numerically determine, only by including a *local Ising* perturbation such as H_inh in eq. (1) can a strong pairing of holes be obtained (see fig. 1). All the calculations were made using exact diagonalization in small clusters with periodic boundary conditions in all spatial directions. We studied one-dimensional (1D) chains

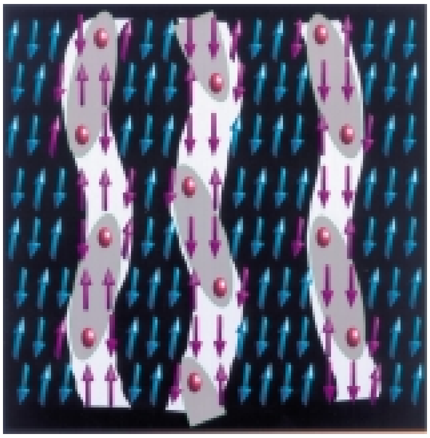

Fig. 1 – Schematic representation of the superconducting ground state. AF zones between stripe segments are colored in blue. Red spins near the stripes represent easy-axis Ising-like links. Gray ellipses characterize the bound pairs (holes in red). Note the zig-zag alignment of the holes, and the AF domains π-shifted at each side of the stripes.

up to 16 sites and 8×2 clusters. Hereafter, we will view our clusters as simulating systems where the longer direction is perpendicular to the stripes. We investigated the system size scaling for the binding energy of two holes defined as $E_{\mathrm{b}} = (E_{2\,\mathrm{holes}} - E_{0\,\mathrm{hole}}) - 2(E_{1\,\mathrm{hole}} - E_{0\,\mathrm{hole}})$ for several models in 1D and 2D. Although for small enough systems the binding energies could be very large, they all seem to extrapolate towards no (or extremely small) binding in the thermodynamic limit, with the clear exception of the inhomogeneous t-JJ_z case. We have also studied several one-band HMs, but we could again not find definite binding. The t-JJ_z model, the only one unambiguously giving binding in the thermodynamic limit, is obtained by breaking spin-rotation symmetry in d near-neighbor bonds $\langle \alpha, \beta \rangle$, repeated with period P, by an amount $\delta J_z = 0$, $\delta J_\perp < 0$ in eq. (1). This t-JJ_z model is a most natural way to induce a spin-gap. We have checked that the spin-gap is present for our t-JJ_z model [13]. The inhomogeneities forming the superstructure, which we impose by hand in the Hamiltonian, we term *stripes*. In fig. 2 we show the hole correlation function $\langle g|n_0 \cdot n_i|g\rangle$, where $|g\rangle$ is the ground state of the system ($\langle g|g\rangle = 1$). This correlation function gives information about the structure of the pair. It can be seen that as the hopping strength t is increased beyond a characteristic value the second hole jumps from one stripe to the neighboring one, starting from an initial configuration where both holes are in the same stripe for small t. This can be understood as a result of a length(time)-scale competition: the pair size exceeds the stripe width.

To explore the nature of the binding, we have examined the canonical transformation of a t-J model from a one-band HM and traced what kind of perturbations would produce a t-JJ_z term. This corresponds to a term like $-V \sum_\sigma \bar{n}_{i,\sigma}\bar{n}_{j,\bar{\sigma}}$ (i, j first neighbors) in an extended HM, which may in turn arise, for example, from local magnetoelastic (*e.g.*, oxygen (un)buckling) [14] or spin-orbit couplings. Note, again, that here this is a perturbation *only* at the stripes. This kind of anisotropy manifests itself in two different ways in the t-JJ_z model, enhancing both the $-\frac{1}{4}\bar{n}_i\bar{n}_j$ and the easy axis (Ising) terms of the Hamiltonian. The first one is an explicit pairing term for *electrons*. To see the relative importance of each term we have calculated the binding energy of a Hamiltonian like (1) but excluding the $-\frac{1}{4}\bar{n}_i\bar{n}_j$ term and including bonds with broken spin-rotational symmetry. This model corresponds to holes (with no spin) propagating in an antiferromagnet, but not derived from a canonical transformation of a one-band HM. We find that it still has binding, as should be expected. Thus, the easy

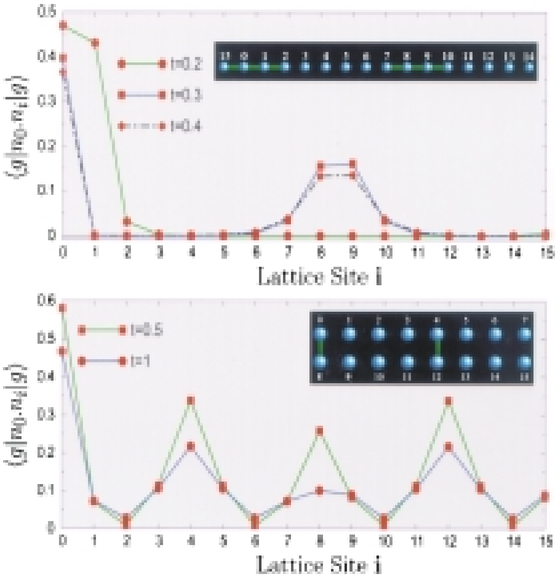

Fig. 2 – Correlation function for 2 holes in a 16×1 chain with $d = 3$, $P = 8$, $J = 1$ and $\delta J_\perp = -0.9$ (top); and for 4 holes in $8{\times}2$ with $d = 1$, $P = 4$ and the other parameters as before (bottom). Lines in the insets show the perturbed bonds. In 16×1, as t grows the pair switches from occupying one single stripe, to two neighboring ones. In the (2 stripes) 8×2 case, the holes remain at both ends of the anisotropic bond, but as t is increased they form an effective two-site stripe because of transverse spin fluctuations. The magnetic energy is lowered by π-shifting the AF domains on either side of the stripe.

axis exchange term is partially responsible for the binding energy.

In order to understand this exchange-based pairing mechanism, it is useful to explore some limiting cases. When the magnetic energy scales are the most relevant ones: ($J_z = J + \delta J_z$, $J_\perp = J + \delta J_\perp$) $\gg t$, it is easy to realize that, depending upon $J_z, J_\perp$ being smaller or larger than J, the holes will prefer to be in the stripes or between stripes (with no binding), respectively. The opposite limit, *i.e.* purely kinetic energy, leads to delocalized holes and no binding. The situation where $J_z < J$ and t is relevant corresponds to the intermediate regime where pairing is observed. Notice that pairing of holes does not necessarily imply that holes should share the same stripe, they can occupy neighboring ones (see fig. 2, upper panel), thus avoiding phase separation. Details of the charge confinement and pairing potentials from the (dynamic) spin-field profiles in the superlattice skeletons will be given elsewhere.

Having demonstrated a minimal model for hole binding, we have computed spin correlation functions in clusters of size $N_x \times N_y = N$ ($N_x = 8, N_y = 2$). Here, we simulate the stripes by including an anisotropic $\delta J_\perp < 0$ in one y-bond with $P = 4$; the rest of the bonds, including all the x-bonds, were not changed from the background t-J model (see inset, fig. 3). We cannot perform scaling on this size of inhomogeneous system, but the binding energy is still considerable. We have included up to 6 holes. In the case of four holes (the one more relevant to the stripes in the underdoped regime for cuprate oxides) and small t ($\lesssim J$) the holes bind in pairs on each site of the inhomogeneous bond (see fig. 2, lower panel).

In fig. 3 we show the spin-structure factor function $S(\boldsymbol{k} = (k_x, k_y))$ defined as $\langle S_{\boldsymbol{k}} S_{-\boldsymbol{k}} \rangle = (1/N) \sum_{\boldsymbol{i},\boldsymbol{j}} \exp[i\boldsymbol{k}\cdot\boldsymbol{r_i}] \, \langle g|\boldsymbol{S_j}\cdot\boldsymbol{S_{j+i}}|g\rangle$. This function corresponds to the observable in the elastic neutron scattering experiments. For t small, only one peak occurs with $k_y = \pi$, corresponding to two essentially uncorrelated AF domains, isolated from each other by the pinned hole wall. As t increases ($t/J \gtrsim 2$, near the accepted set of values of the 2D t-J model for cuprates [15]),

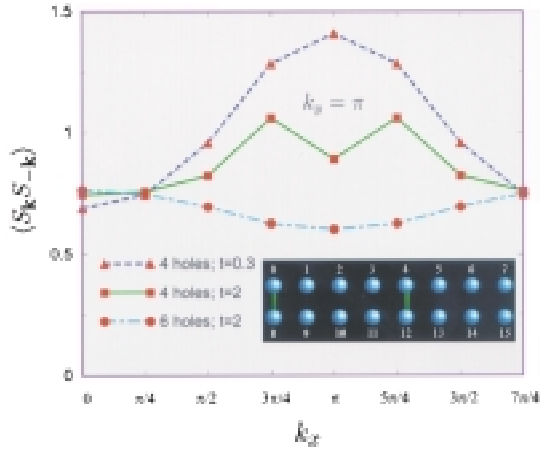

Fig. 3 – Spin-structure factor for a t-JJ_z ladder (8×2) with two $\delta J_\perp = -0.9$ bonds in the y-direction (see inset). The incommensurability appears only for t larger than a critical value. When 6 holes are added to the system the double peak disappears and is replaced by a broad one around $\boldsymbol{k} = (0, \pi)$.

the holes gain kinetic energy by visiting the first neighbor sites around the anisotropy region, but still bind together. The effective width of the pair thus increases to two sites. Magnetic energy is then gained if the two domains shift their staggered magnetization by π. We suggest that these $\mathcal{O}(t^2)$ processes are responsible for the incommensuration (δ) in $S(\boldsymbol{k})$ observed in the experiments [1]. This δ is the inverse of twice the period P of the stripes. In this picture the incommensuration is a consequence of the holes and their kinetic energy, and is a property of the ground state. Basically, it results from the competition between hole delocalization and magnetic fluctuations. This contrasts with some other proposed explanations, where δ is a magnetic thermodynamic property [16]. It is interesting to note that this incommensuration arises even in the homogeneous t-J model although for different values of t. This suggests that the experimentally observed magnetic properties are already present in a homogeneous t-J model, but in order to obtain binding of holes appropriate inhomogeneous terms must be included.

When more than four holes are added to the system, but only two bonds are perturbed, $S(\boldsymbol{k})$ changes qualitatively. Instead of showing an incommensurability around $\boldsymbol{k} = \boldsymbol{Q} = (\pi, \pi)$, it has a broad peak at $\boldsymbol{k} = (0, \pi)$. In this case the extra holes are delocalized in the middle of the AF space between stripes. This suggests that when the stripes reach their minimum separation, extra holes are responsible for the experimental increase and ultimate disappearance of the incommensurability.

Model of Josephson spaghetti. – It is important to relate the above discussion to the experimental evidence for the incommensurate neutron scattering peak, seen in LSCO (*e.g.*, [3]) and YBCO compounds [2]. In both of these cases a simple *linear* relation between T_c and the peak incommensuration δ near $\boldsymbol{Q}$ (or peak width in YBCO) is obeyed [3, 4]. Namely,

$$k_\mathrm{B} T_\mathrm{c} = \hbar v^* \delta \ . \tag{2}$$

The anomalously low velocity values for v^* depend on the compound [4]. These velocities are independent of the carrier concentration and the only doping (x) dependence entering eq. (2) is through $\delta(x)$.

An interpretation of this relation is to connect possible superconductivity mechanisms to the existence of the fluctuating stripes. Here we focus on the simple proportionality between $T_\mathrm{c}(x)$ and a doping dependent length $\ell(x)$, determined from the neutron scattering:

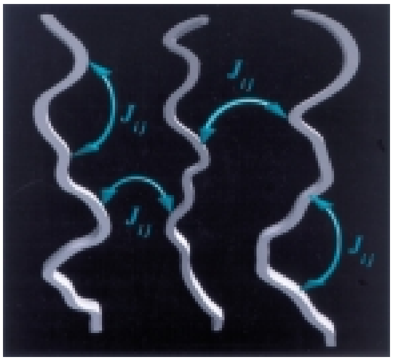

Fig. 4 – Schematic Josephson coupling between an assumed distribution of stripe segments. For the incommensuration δ to be observed along crystallographic (1,0) and (0,1) directions, the stripe-stripe distances must have average $\langle r\rangle \approx \ell = 1/\delta$. $\langle J\rangle$ will be determined by the probability distribution $P(r)$ that determines the statistics of inter-stripe distances. Physically it is clear that $P(r)$ should be centered near ℓ, with some width arising from the meandering of stripes (see text).

$T_{\mathrm{c}}(x) \propto 1/\ell(x)$, $\ell(x) = 1/\delta(x)$. We consider how the Josephson tunneling of pairs between stripe segments can produce the relation between the phase ordering transition temperature T_{c} and the typical length $\ell(x)$. The stripe-stripe distance r is a random quantity due to intrinsic mechanisms as well as disorder and/or crystal imperfections [11, 12]. Therefore, we will assume that the mean-field transition temperature depends upon the Josephson coupling $\langle J(r)\rangle$, averaged with some probability distribution of stripe separations.

Our model Hamiltonian of random stripe separation and associated inter- and intra-stripe random Josephson coupling (see fig. 4) is

$$\mathcal{H} = \sum_{ij} J_{ij}\ \exp[i(\phi_i - \phi_j)]\ , \qquad J_{ij} = J(r_{ij}) = t_0/r_{ij}^{\alpha}\ , \tag{3}$$

where the summation is taken over the coarse-grained regions $i = 1, \cdots, \mathcal{N}$ with well-defined phases, labeled $\phi_i = \phi(r_i)$ and J_{ij} becomes zero eventually at large distances. Next, we will assume some probability distribution $P(r)$ for the stripe-stripe distance. For simplicity we will take the "box" distribution $P(r)$ centered around $\ell = 1/\delta$ and with finite width $a = \nu\ell$, where $\nu = \mathcal{O}(1)$ is a parameter. $P(r) = C$, for $\ell - a \leq r \leq \ell + a$, and zero otherwise. Here we have simplified to one length scale for both a and ℓ. The normalization constant in 2D is $C = [4\pi\ell a]^{-1}$. In this model one easily finds

$$\begin{aligned} \langle J(r)\rangle &= \int \mathrm{d}^2 r P(r) J(r) = \frac{2\pi t_0 C}{2-\alpha} a_1 \ell^{2-\alpha}\ , \\ \langle r\rangle &= \frac{2\pi C}{3} a_2 \ell^3\ , \end{aligned} \tag{4}$$

where the constants a_1, a_2 are $\mathcal{O}(1)$. Thus, for $\alpha = 1$, we obtain the experimentally observed relation

$$T_{\mathrm{c}}(x) \simeq \langle J(r)\rangle \propto [\langle r\rangle]^{-1} = \delta(x)\ . \tag{5}$$

We have examined a variety of distributions $P(r)$ and functional dependences for J_{ij}; eq. (3) with $\alpha = 1$ is the only one reproducing the experimental data (at our mean-field random Josephson coupling level. Implicit in $J(r)$ is the exponential cutoff at lengths much larger than the stripe-stripe distance. This cutoff is necessary to have a well-defined thermodynamic limit but is not important for short length scales). The screening mechanism (magnetic, elastic fluctuations, etc.) responsible for this form requires detailed microscopic modeling [17]. The present model does not allow us to determine the magnitude of v^* without making specific assumptions about parameters such as t_0.

In conclusion, we have presented a microscopic model that captures the essential magnetic and pairing properties of high-temperature cuprate superconductors. Pairing of holes is a consequence of the existence of an AF background. (Analogous scenarios in other broken symmetry backgrounds, *e.g.*, doped charge-density-wave bismuthates, are likely.) Crucially, however, the glue is provided by magnetic *inhomogeneities* whose precise origin remains to be unraveled, although it seems fundamental that these perturbations should *locally* break spin-rotational invariance. This pairing mechanism is kinetic exchange-interaction–based and involves a competition between Ising and XY symmetries. We emphasize that the pair-binding occurs only for intermediate strengths of t and (local) J_z. We also introduced a phenomenological model and scenario for the macroscopic superconductivity based upon coherent Josephson-tunneling of pairs of holes between these magnetic inhomogeneities in a mesoscopic liquid-crystal–like [11] skeleton. We have shown that this approach is able to recover the magnetic incommensuration δ and its experimentally observed relation to $T_c(x)$. Finally, we note that we have assumed static magnetic inhomogeneities. The case where the broken spin-symmetry follows the hole is also interesting. Elsewhere, we will discuss this generalization of coupling the inhomogeneity self-consistently to dynamic holes.

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Work at Los Alamos is sponsored by the US DOE under contract W-7405-ENG-36.

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